

Pentanedioic acid, 3,3-dimethyl-
4839-46-7 | DTXSID9063617

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 4.27×10^{-12} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 4.41×10^{-1}

Confidence level: 7.62×10^{-1}

Nearest Neighbors from the Training Set

Image not found

Dimethyl adipate

Measured: 8.40×10^{-12}

Predicted: 6.84×10^{-12}

Image not found

Dimethyl glutarate

Measured: 3.30×10^{-12}

Predicted: 3.76×10^{-12}

Image not found

Dimethyl succinate

Measured: 1.40×10^{-12}

Predicted: 1.93×10^{-12}

Image not found

2-Ethoxyethyl isobutyrate

Measured: 1.35×10^{-11}

Predicted: 1.28×10^{-11}

Image not found

Ethyl lactate

Measured: 3.90×10^{-12}

Predicted: 4.80×10^{-12}